Green's function Monte Carlo Calculations of Light Nuclei

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Work with

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K. Varga, Oak Ridge

Work not possible without

Math & Computer Science Division Computers

(Est. 900K CPU-hours $\approx$ 110 TFLOP hours in FY01)

NERSC IBM SP

(963K charge hours = 385K CPU-hours

$\approx$ 135 TFLOP hours in FY01)

Two Problems in Microscopic Few- & Many-Nucleon Calculations

(I) What is the Hamiltonian?

- NN force is reasonably controlled
- 3N force must be determined while computing properties of light nuclei!

(II) Given $\mathcal{H}$, solve the Schrödinger equation for A nucleons accurately.

- Much recent progress for $A \leq 10$

Direct comparison of calculations to data is ambiguous if (II) is not solved.

Our goal is a microscopic description of nuclear structure and reactions from bare NN & 3N forces and consistent currents.

Nuclear Hamiltonian

$$\mathcal{H} = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

v_{ij}: Argonne v_{18}

$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{CS} + v_{ij}^{CD}$ $v_{ij}^{CS} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^{p}$

$O_{ij}^{p=1,14} =$

$[1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L}\cdot\mathbf{S}, \mathbf{L}^2, \mathbf{L}^2\sigma_i\cdot\sigma_j, (\mathbf{L}\cdot\mathbf{S})^2] \otimes [1, \tau_i \cdot \tau_j]$

V_{ijk}: Urbana IX and new Illinois models

Need to solve

$$\begin{aligned} &\mathcal{H}\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_a; t_1, t_2, \cdots, t_A) \\ = &E\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_a; t_1, t_2, \cdots, t_A) \end{aligned}$$

s_i are nucleon spins: $\pm\frac{1}{2}$

t_i are nucleon isospins (proton or neutron): $\pm\frac{1}{2}$

$2^A \times \begin{pmatrix} A \\ Z \end{pmatrix}$ coupled equations in $3A$ variables

(number of isospin states can be somewhat limited)

Variational Monte Carlo

Minimize expectation value of $\mathcal{H}$

$$E_T = \frac{\langle \Psi_T | \mathcal{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

Simplified trial wave function:

$$|\Psi_T\rangle = [1 + \sum_{i<j<k} U_{ijk}][\mathcal{S} \prod_{i<j} (1 + U_{ij})] \prod_{i<j} f_{ij} |\Phi\rangle$$

U_{ijk} are 3-body correlations from V_{ijk}
U_{ij} are non-commuting 2-body correlations from v_{ij}
f_{ij} are central (mostly short-ranged repulsion) correlations

Φ is a $1\hbar\omega$ shell-model w.f.

- determines quantum numbers of state
- fully antisymmetric
- translationally invariant
- has multiple spatial-symmetry components

Green's Function Monte Carlo

VMC Ψ_T propagated to imaginary time τ:

$$\begin{aligned} \Psi(\tau) &= e^{-(\mathcal{H}-E_0)\tau}\Psi_T \\ \Psi_0 &= \lim_{\tau\to\infty}\Psi(\tau) \\ \mathcal{H}\Psi_0 &= E_0\Psi_0 \end{aligned}$$

Small time-step propagator:

$$\Psi(\tau) = \left[e^{-(\mathcal{H}-E_0)\triangle\tau}\right]^n \Psi_T; \quad \tau = n\triangle\tau$$

$$G_{\beta\alpha}(\mathbf{R}',\mathbf{R}) = \langle\mathbf{R}',\beta|e^{-(\mathcal{H}-E_0)\triangle\tau}|\mathbf{R},\alpha\rangle$$

$\Psi(\mathbf{R}_n,\tau) =$
$\int G(\mathbf{R}_n,\mathbf{R}_{n-1})\cdots G(\mathbf{R}_1,\mathbf{R}_0)\Psi_T(\mathbf{R}_0,0)d\mathbf{R}_{n-1}\cdots d\mathbf{R}_0$

Fermion sign problem limits maximum τ:
G brings in lower-energy boson solution
$\langle\Psi_T|\mathcal{H}|\Psi(\tau)\rangle$ projects back fermion solution
Exponentially growing statistical errors

Constrained-path propagation, suggested by J. Carlson, removes steps that have

$$\overline{\Psi(\tau,\mathbf{R})^\dagger\Psi(\mathbf{R})} = 0$$

Many tests demonstrate reliability

Making It Parallel

Master-slave structure

Each slave gets configurations to propagate

Results sent back to master for averaging as generated

During propagation, configs multiply or are killed

- Work load fluctuates
- Periodically master collects statistics and tells slaves to redistribute
- Slaves have work set aside to do during this synchronization

Large calculations have very low (minutes) frequency of communication

Parallelization efficiencies typically 95%

92% efficency obtained on 2048-processor Seaborg run; 0.55 TFLOPS.

Typical Current Calculations

- Propagation to $\tau = 0.2 - 0.4$ MeV^{-1}
- $E(\tau)$ every $\tau = 0.01$ MeV^{-1} (0.02 for $A \geq$10)
- Average of $E(\tau)$ for $\tau \geq 0.1$

	Config-urations	τ_{max} MeV^{-1}	Statistical Error (MeV)	Processor hours*
^{6}Li	50,000	0.2	0.08	40
^{7}Li	20,000	0.2	0.14	340
^{8}Be	15,000	0.2	0.2	300
^{8}Li	12,000	0.2	0.2	600
^{9}Be	6,500	0.4	0.5	10,000
^{9}Li	8,000	0.4	0.4	13,500
^{10}B	5,000	0.5	0.5	5,000
^{10}Be	3,000	0.6	0.6	9,000

*6 – 8: IBM SP3 or SGI 250 MHz R10000 processors
9: 500 MHz Pentium-III at ~ 110 MFLOPS (MCS Chiba City)
10: IBM SP at ~ 320 MFLOPS (NERSC Seaborg)

^{3}H$(\alpha,\gamma)^7$Li & ^{3}He$(\alpha,\gamma)^7$Be Capture Reactions

U. of Chicago thesis work of K. Nollett

Source of ^{7}Li in the big bang

- Astrophysically important region is 20−500 keV.

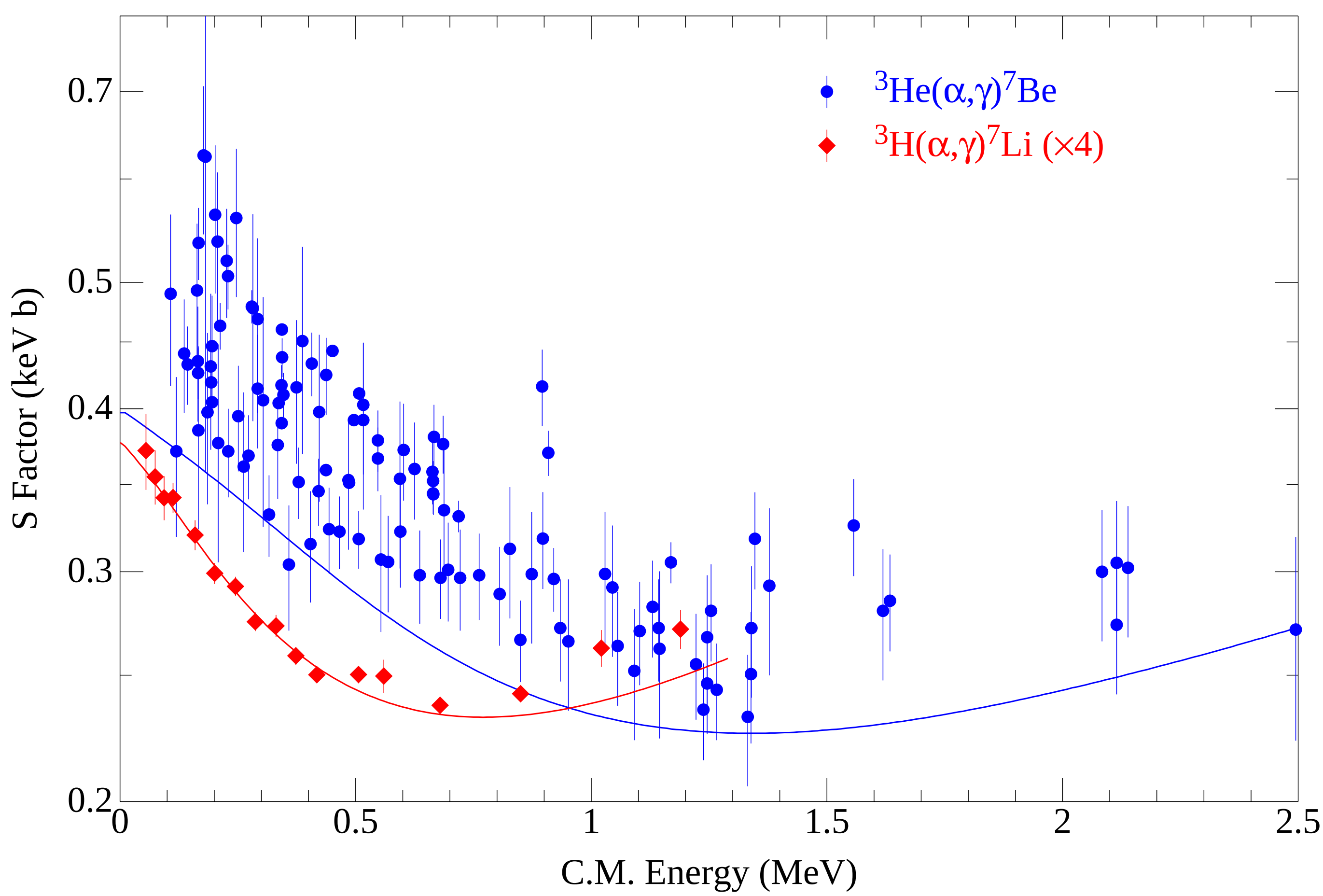
^{7}Be reaction also source of solar neutrinos

- Astrophysically important region is 20 keV.
- No data in this region

Full 7-nucleon calculation

- $A = 7$ wave functions have proper 3+4 cluster form.

^{2}H$(\alpha,\gamma)^6$Li also done



Recent Progress

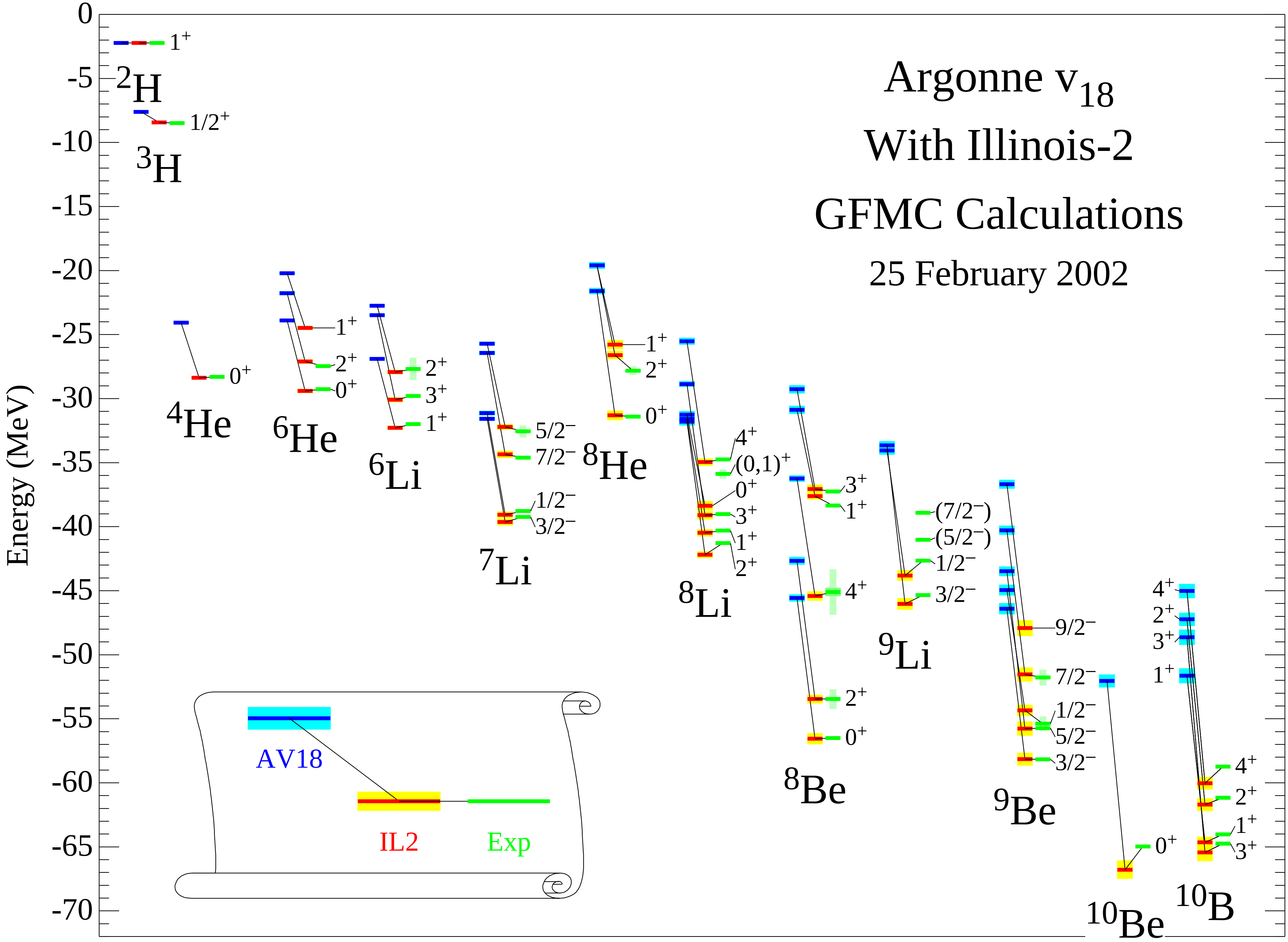
- New computers and methods allow $\sim 1 - 2\%$ calculations of light p-shell nuclear energies
- First $A =$ 9,10 calculations done in FY2000. Full set done in 2001 to early 2002
- First $A = 10$ unnatural-parity states done in FY2001
- Extensions to the Urbana V_{ijk} give average binding-energy errors < 0.7 MeV for $A = 3 - 10$ nuclei
- Variational w.f. with proper asymptotic clustering
- VMC calculations of weak transitions in $A = 6, 7$
- Participated in ^{4}He benchmark paper using seven precise methods; GFMC good to $\leq 0.1\%$ for AV8$'$
- Study of what is needed in nuclear potentials to get observed nuclear level structure

Plans

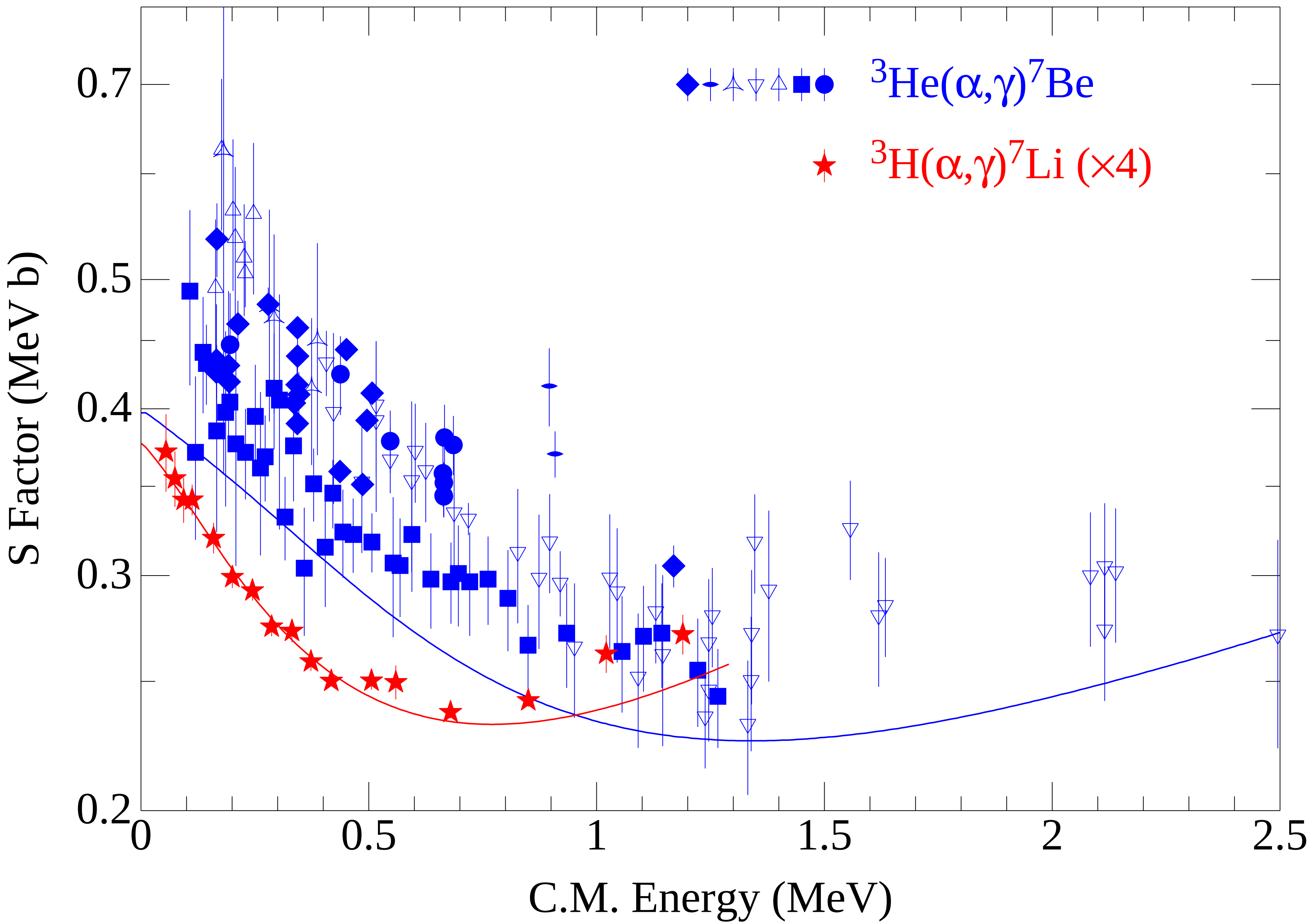
- GFMC for scattering states – widths of resonances
- $A = 9,10$ – continue study of intruder states
- ^{7}Be(p,γ)^{8}B, ^{8}B(β^{+})^{8}Be, ^{9}Be(e,e$'$N), ^{10}C(β^{+})^{10}B, ...
- neutron-rich systems – input for large-nuclei methods
- ^{12}C by GFMC (several years away)

We are approaching a nuclear standard model for computing nuclear properties and reactions

GFMC calculations are the benchmark for $6 \leq A \leq 10$



Argonne v18
With Illinois-2
GFMC Calculations
25 February 2002
Energy (MeV)
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
2H
1+
3H
1/2+
4He
0+
6He
1+
2+
0+
6Li
2+
3+
1+
7Li
5/2−
7/2−
1/2−
3/2−
8He
1+
2+
0+
8Li
4+
(0,1)+
0+
3+
1+
2+
8Be
3+
1+
4+
2+
0+
9Li
(7/2−)
(5/2−)
1/2−
3/2−
9Be
9/2−
7/2−
1/2−
5/2−
3/2−
10Be
0+
10B
4+
2+
3+
1+
4+
2+
1+
3+
AV18
IL2
Exp



S Factor (MeV b)
C.M. Energy (MeV)
0.2
0.3
0.4
0.5
0.7
0
0.5
1
1.5
2
2.5
^{3}He(α,γ)^{7}Be
^{3}H(α,γ)^{7}Li (×4)